Characterizing Large-Scale Computational Physics

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Biases

- **Intentional**
  - Large-scale
- **Inevitable**
  - Department of Energy
    - NERSC
    - Advanced Computing Laboratory (LANL)
    - Argonne Leadership Computing Facility
  - Plasma physics
  - USA

Questions

- **Is it physics?**

Lattice QCD | Molecular dynamics | Protein folding

Plasma simulation | Electronic Structure

Physical Review | *J. Chem. Phys.*

- **Is it large-scale?**
  - 20% of leadership-class machine
  - Distributed-memory parallelism
  - Too large/slow for O(100) processor cluster

Sources

- **Journals**
  - *Physical Review*
  - Journal of Computational Physics
  - IEEE Computer
- **Proceedings**
  - SC, IPDPS
  - Extreme Scale workshops
- **Computer center annual reports**
  - NERSC, ALCF, OLCF, PSC, TACC
- **Reviews/reports**
  - SciDAC Review
  - Computation as a Tool for Discovery in Physics (NSF report, 2002)
- **Books**
  - *Petascale Computing: Algorithms and Applications* (Bader, 2008)
  - Various “Computational Physics” texts

Physics Areas

Condensed Matter	High Energy	Astrophysics/ Relativity
Plasma	Atomic/Molecular	Nuclear
Climate/weather	Turbulence	Geophysics
…		

Application Types

- Lattice QCD
- Electronic Structure
  - DFT
- Electromagnetics
- Accelerator Beam
- Monte Carlo Transport
- Climate
- Nuclear Structure
- Combustion
  - Nuclear Burn
  - DDT
- Plasma
  - PIC
  - Kinetic
  - Fluid(s)
- CFD
  - DNS
  - Lattice Gas/Boltzmann
  - LES/RANS
  - SPH
- Cosmology Structure Evolution
- Structural Mechanics
- Earthquake
  - Seismic Wave Propagation
  - Dynamic Rupture
- Atomistic Molecular Dynamics

Wide Range of Scales of Interest

Turbulence

Wide Range of Scales

Turbulent Fluid Flow.

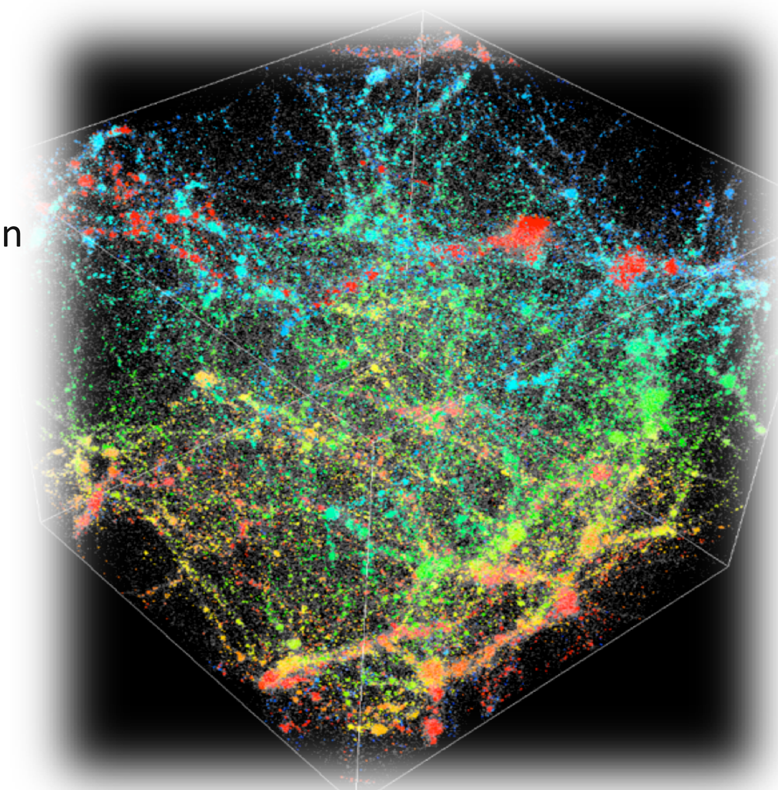
- **Range of length scales in 3D turbulence ~ $R_e^{9/4}$**
- **State-of-the-art DNS (direct numerical simulation): $R_e = O(10^4)$**
  - Range of length scales = $O(10^9)$
- **Need for more**
  - Physical R_e for commercial jet aircraft = $O(10^7 – 10^8)$
  - Physical R_e for atmospheric flow = $O(10^7 – 10^8)$

Cosmology

Wide Range of Scales

Cosmology: Simulate evolution of large-scale structure of the universe

- **State-of-the-art simulation: resolve galaxy-halo-sized structures**
- **Range of length scales is > 10^5**
  - Simulation domain 1 Gpc on a side
  - Force resolution O(10) kpc
- **Range of mass scales is 10^4-10^5**
  - 1 ptcl is 1-10 billion M_{sun}
  - Milky Way dark matter halo is 60 billion - 3 trillion solar masses
  - 10 billion ptcles

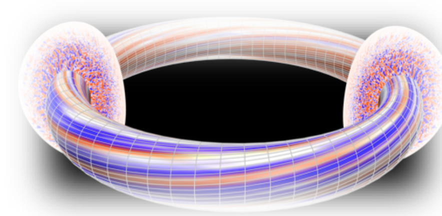


- **Need for more**
  - Resolve galaxies ("baryonic" matter)…stars

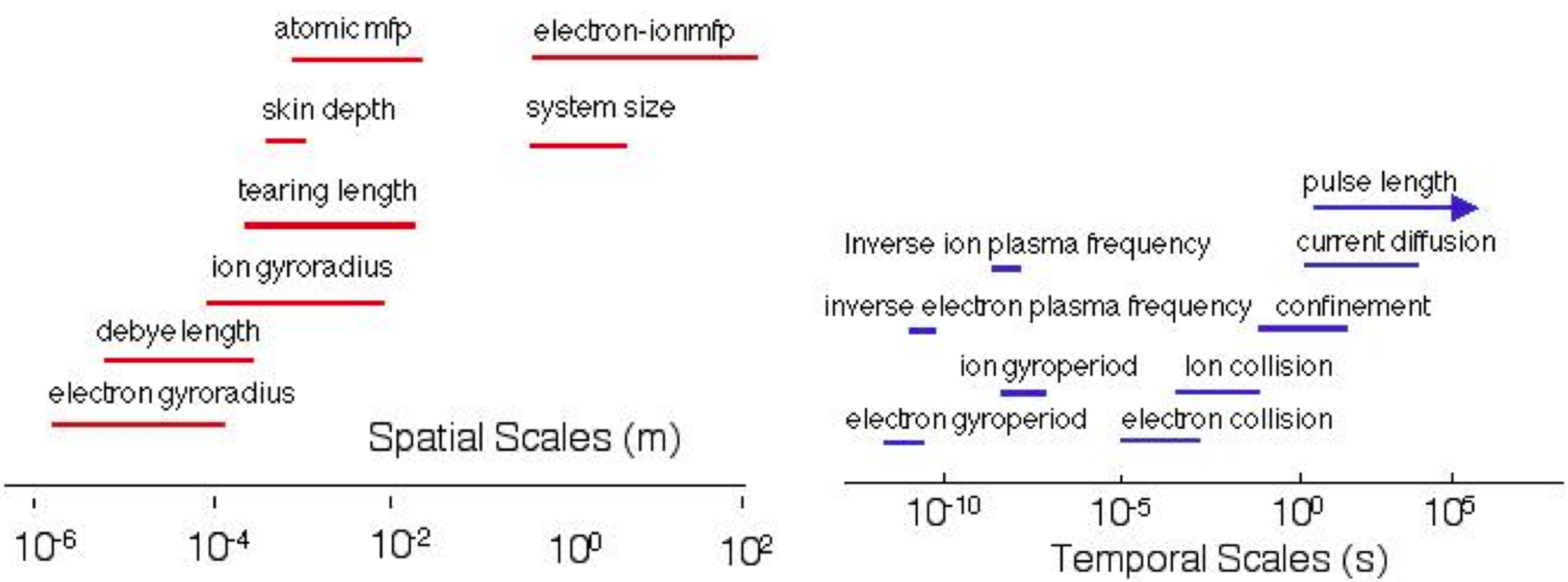
White, et al., Astrophysical J. 713 (2010) 383 (http://iopscience.iop.org/0004-637X/713/1/383).
Figure: Habib, ALCF Early Science Kick-Off Workshop (http://workshops.alcf.anl.gov/esp10/agenda/)

Plasma Physics

Wide Range of Scales



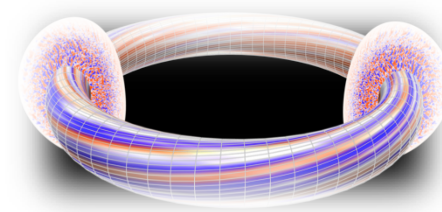
Fusion energy applications.



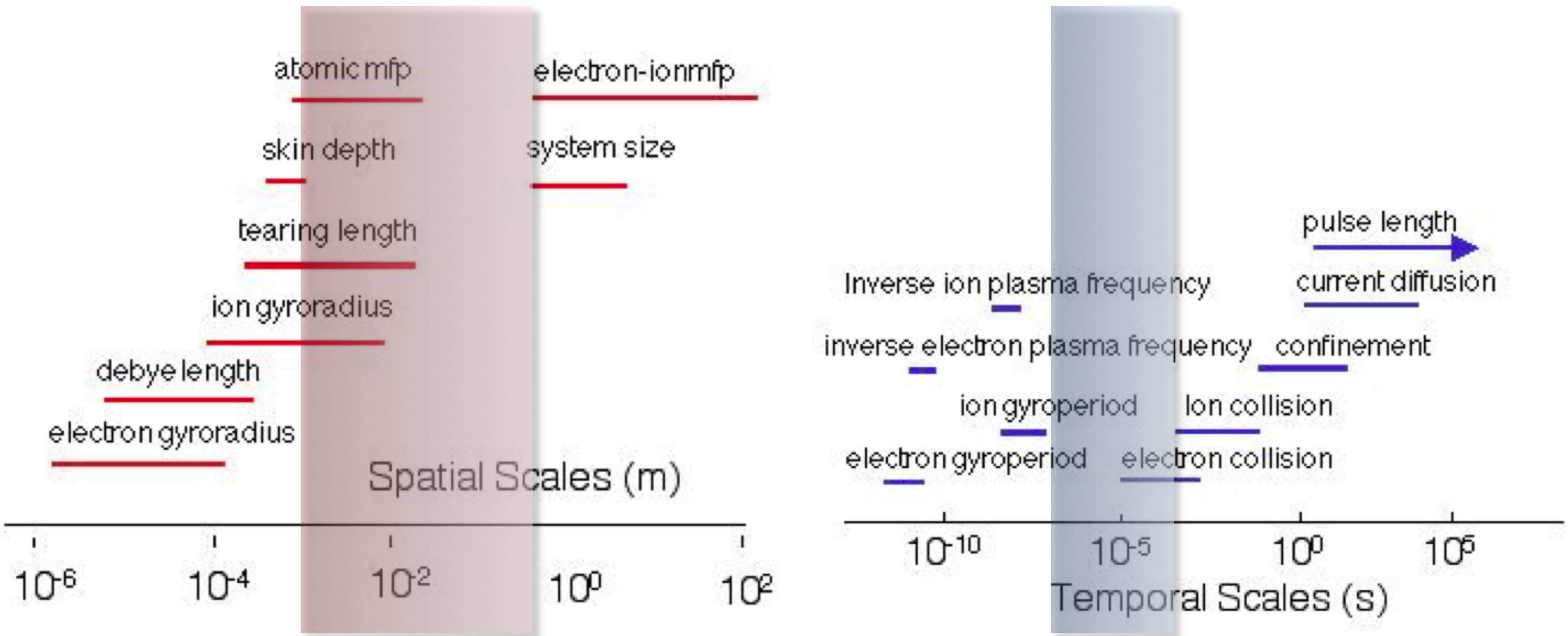
Cui et al., "Scalable Earthquake Simulation on Petascale Supercomputers," SC10, vol., no., pp.1-20, 13-19 Nov. 2010. (http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=5644908&isnumber=5644843)

Plasma Physics

Wide Range of Scales



Electrostatic ion microturbulence in a tokamak



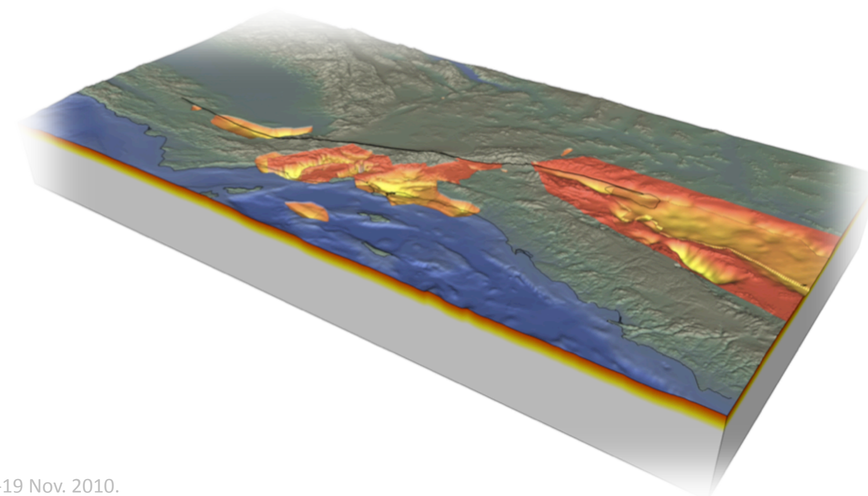
- **Need for more**
  - Electron kinetics, full-*f*
  - Magnetic fluctuations

Geophysics

Wide Range of Scales

Seismic Wave Propagation.

- **State-of-the-art simulation**
  - M8: magnitude-8 on San Andreas Fault
    - 800 x 400 km area in Southern California (85 km deep)
    - Frequencies 0-2 Hz
    - 6 minutes simulated time
    - Grid resolution 40 m ==> 436 billion grid cells
    - CFL ==> 160,000 timesteps
- **Need for more**
  - Sub-skyscraper building relevance: 3-10 Hz



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Brute Force Computational Approach

Turbulence

Brute Force Approach

Turbulent Fluid Flow.

- **Direct Numerical Simulation: Discrete solution of Navier-Stokes equations**
  - Finite volume
  - Spectral
  - Pseudospectral
  - Spectral element

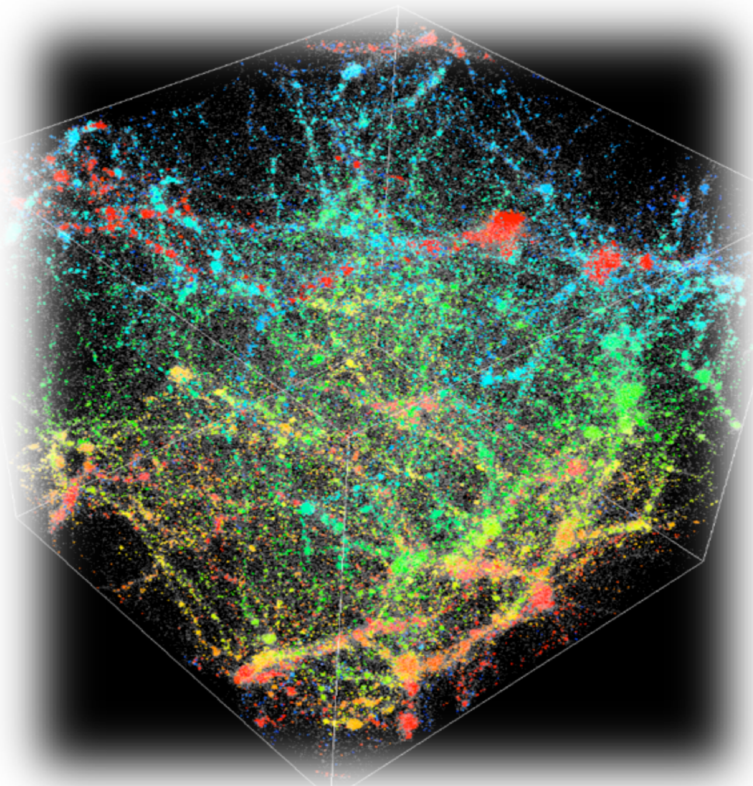
- **Less brutish, but less general**
  - Reynolds-averaged Navier-Stokes (RANS)
  - Large-eddy simulation (LES)

Cosmology

Brute Force Approach

Simulate evolution of large-scale structure of the universe.

- **Dark matter: Particle-mesh**
  - Poisson solve for long-range interactions
  - Short-range interactions
  - **MC^3** code: local particle-particle interaction
  - **Enzo** code: AMR



Plasma Physics

Brute Force Approach

Fusion energy applications: tokamak ion microturbulence

- **Ions: Vlasov equation for phase-space distribution *f(x,p)***
  - Reduce to *gyrokinetic* form representing sufficient
  - **GTC** code: particle-in-cell (PIC) ions
  - **GYRO** code: discretize (**x**,**p**) phase space
- **Electromagnetic fields: Maxwell's equations**
  - Reduce to Poisson equation in electrostatic limit

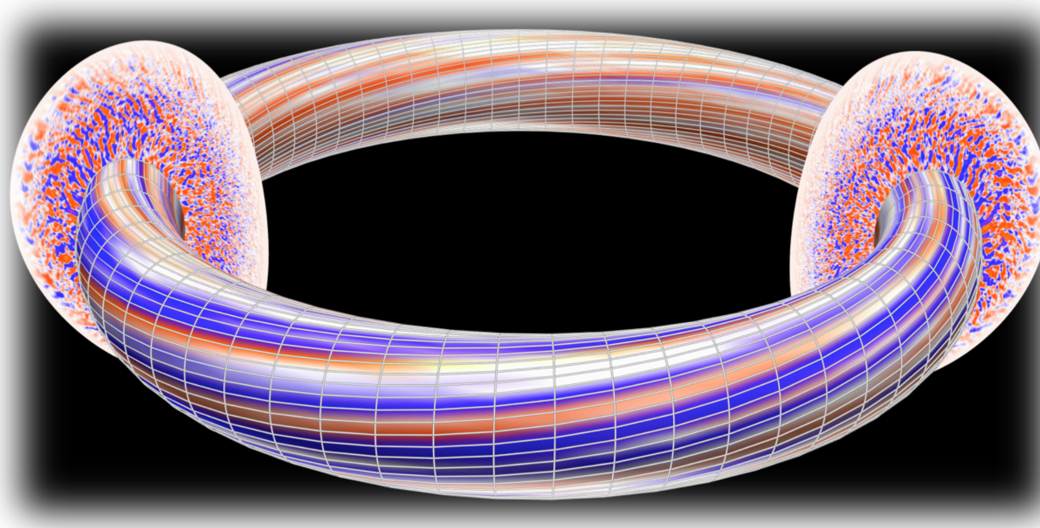


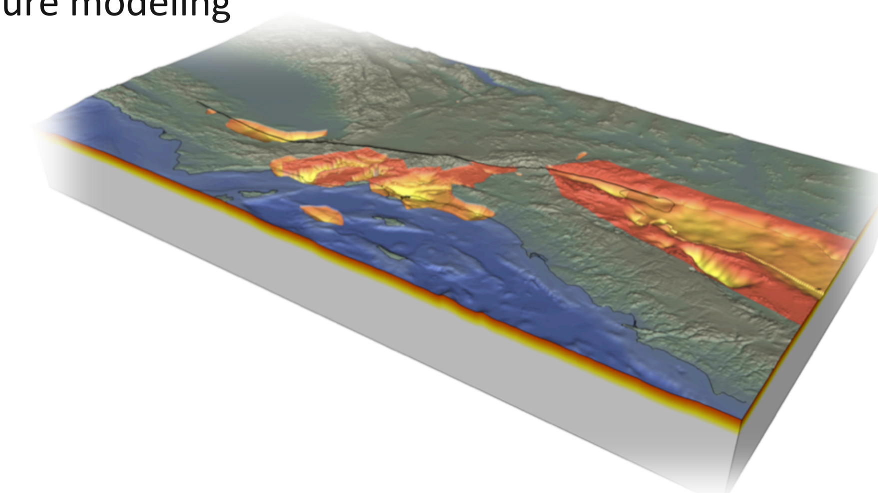
Figure: Tang, ALCF Early Science Kick-Off Workshop (http://workshops.alcf.anl.gov/esp10/agenda/)

Geophysics

Brute Force Approach

Seismic Wave Propagation.

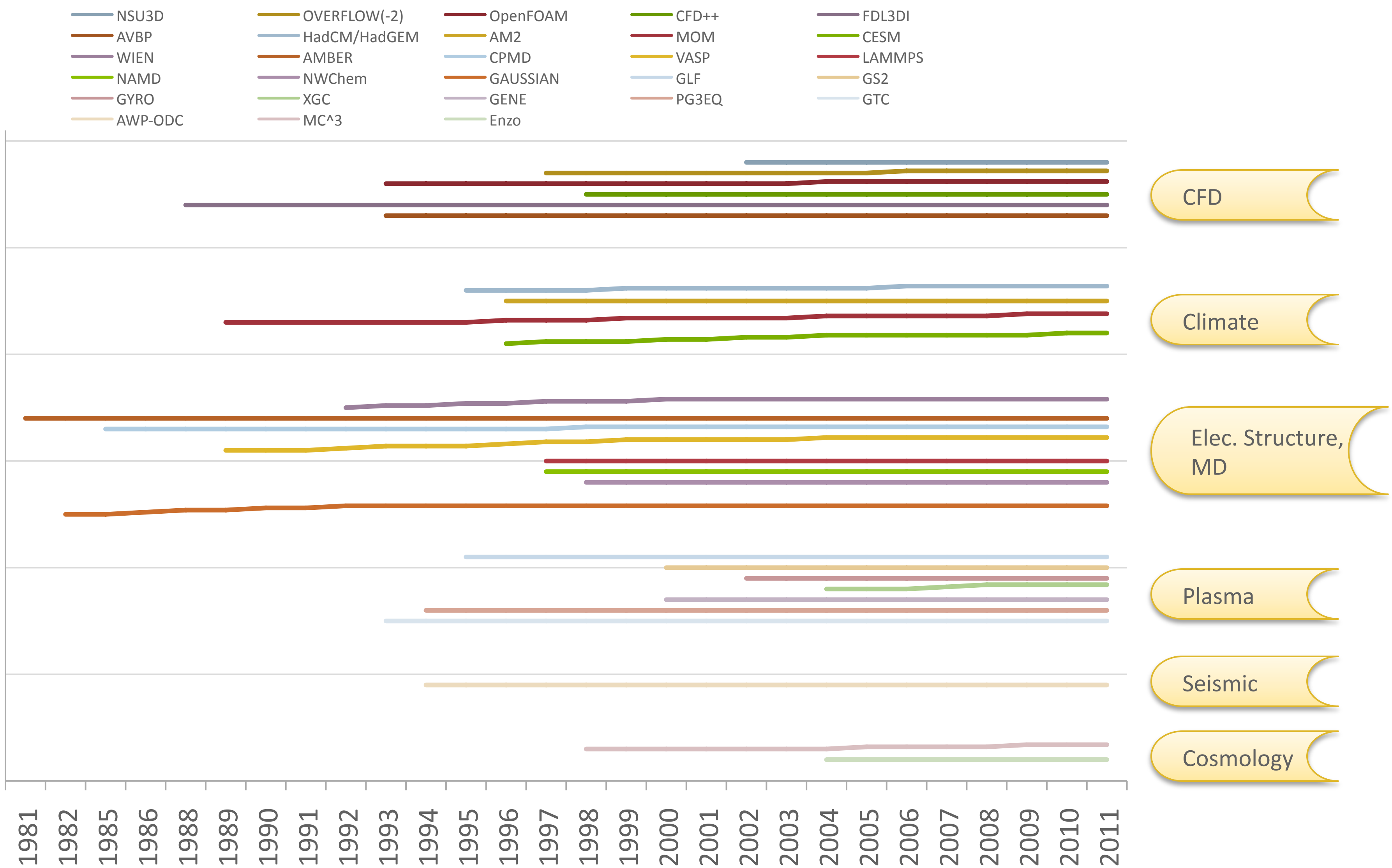
- **Discrete solution of equations for anelastic solids**
  - Finite difference (FD)
  - Finite volume
  - Spectral element
  - Finite element
- **AWP-ODC code: staggered FD scheme**
  - 4^{th} order in space, 2^{nd} order in time
  - Split-node algorithm for dynamic fault rupture modeling
  - M8 problem: uniform mesh



Persistent Players

Live Long

Persistent Players



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Slides: http://www.alcf.anl.gov/~zippy/publications/presentations/APSMarch2011.pdf